Ethyl 7-ethylcinnoline-3-carboxylate

89770-38-7	DTXSID00632289	

Model Performance

Model	Data

Weighted KNN model

5-fold CV	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 7.70e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.26e-01

Confidence level: 4.94e-01

Nearest Neighbors from the Training Set

Image not found

Butyl (2,4,5-

trichlorophenoxy)acetate
Measured: 1.18e-04
Predicted: 2.42e-05

Image not found

Azafenidin

Measured: 1.40e-06 Predicted: 5.75e-11

Image not found

Kinoprene

Measured: 1.50e-08 Predicted: 1.35e-05

Image not found

Tetraconazole

Measured: 3.00e-08 Predicted: 2.75e-06

Image not found

Metobenzuron

Measured: 1.35e-06 Predicted: 2.39e-06